

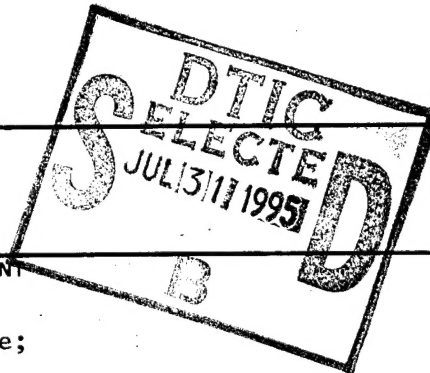
REPORT DOCUMENTATION PAGE

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1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE		3. REPORT TYPE AND DATES COVERED FINAL 01 Jun 92 To 31 May 95	
4. TITLE AND SUBTITLE NEW METHODS FOR TREATMENT OF ELECTRON CORRELATION AND SURFACE DYNAMICS				5. FUNDING NUMBERS F49620-92-J-0244 3484/S2 61103D	
6. AUTHOR(S) Prof. Emily A. Carter					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Dept of Chemistry & Biochemistry University of California, Los Angeles 405 Hilgard Avenue Los Angeles CA 90024-1569				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NL 110 Duncan Ave Suite B115 Bolling AFB DC 20332-0001 Dr Michael R. Berman				10. SPONSORING / MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES					
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; Distribution unlimited.				12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) I have funding to support one student through the AASERT program. Over the past three years, I have split this money between four students, Todd J. Martinez, Lawrence E. Carter, Claudine C. Tazartes, and Michelle R. Radeke. I now briefly describe their research accomplishments related to the AASERT grant. (All of them have more than satisfactory grades and all are U.S. citizens.)					
14. SUBJECT TERMS				15. NUMBER OF PAGES	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED		18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED		19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	
				20. LIMITATION OF ABSTRACT UNCLASSIFIED	



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AASERT Final Technical Report

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June 30, 1995

I have funding to support one student through the AASERT program. Over the past three years, I have split this money between four students, Todd J. Martinez, Lawrence E. Carter, Claudine C. Tazartes, and Michelle R. Radeke. I now briefly describe their research accomplishments related to the AASERT grant. (All of them have more than satisfactory grades and all are U. S. citizens.)

Todd Martinez was the primary student supported on this grant, and he earned his Ph. D. in September 1994. His thesis involved utilizing pseudospectral numerical approaches to the electron correlation problem, with the goal of developing accurate methods that scale better than current analytical methods such that larger molecules can be treated with configuration interaction (CI) or perturbation theory. In the past three years, we have published four papers and one book chapter due to appear this summer (reprints/preprints of which were sent to AFOSR already) on this subject. The first concerned the development of pseudospectral full configuration interaction [*Journal of Chemical Physics*, **97**, 1876 (1992)], the second discussed the creation of pseudospectral double excitation configuration interaction [*Journal of Chemical Physics*, **98**, 7081 (1993)], the third presented pseudospectral many-body perturbation theory through third order [*Journal of Chemical Physics*, **100**, 3631 (1994)], the fourth formulated pseudospectral multireference single and double excitation configuration interaction [*Journal of Chemical Physics*, **102**, 7564 (1995)], and the book chapter is a pedagogical review of pseudospectral electron correlation methods emphasizing its relationship to other approaches (to appear in "Modern Electronic Structure Theory," edited by D. R. Yarkony, in the World Scientific Advanced Series in Physical Chemistry). We have shown that while pseudospectral full CI can be accurate but not practical under today's data storage conditions, truncated CI and perturbation theory calculations in fact show a distinct advantage in scaling while retaining chemical accuracy. For example, we have demonstrated that our pseudospectral MP2 code is an order of magnitude faster than existing commercial codes (Gaussian 92) for moderate-sized molecules with modest basis sets, and is expected to be even faster for molecules with extensive basis sets. Our pseudospectral MP3 code is extremely accurate and also faster than Gaussian 92, with expected speedups of more than an order of magnitude for large molecules. Todd's pseudospectral multireference single and double excitation configuration interaction method for arbitrary spin states turns out to be even more accurate than our MP2 method (average error for a series of molecules is 0.2 kcal/mol in the total energy), and up to six times faster than conventional spectral methods. We are extremely encouraged by the speed and accuracy of these new methods for treating electron correlation that we have developed in the last few years, and expect to continue our development of these methods in the years to come.

Lawrence E. Carter was the second most supported student on this grant. He is finishing up his thesis this summer. He carried out Monte Carlo and ab initio-derived molecular dynamics simulations of SiGe superlattice structures and F₂ and F atom/Si(100) reaction dynamics. Four papers have been published in the last two years, one is about to be submitted for publication, and two more are in preparation (the published papers have been sent to the AFOSR in preprint and reprint form). The SiGe superlattice simulations [*Journal of Vacuum Science and Technology A*, **11**, 2059 (1993)] were designed to ascertain the atomic level structure of Si_xGe_{1-x}/Si and Si_xGe_{1-x}/Ge electronic devices. In addition, we developed a split-box pseudo-constant pressure technique used in this work to allow fast equilibration of two solids in contact with one another. We were interested in comparing the structures near the interface between the SiGe alloy and the pure

